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# Chemistry for Measurement and Detection Science

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### Project Description

Chemistry used in measurement and detection science plays a crucial role in the Laboratory's Science of Signatures scientific thrust.

Measurement and detection science areas that require chemistry include nuclear and radiological, materials, biological, energy, climate, and space.

Los Alamos scientists integrate chemical-science capabilities to ensure that the Laboratory can respond effectively to national emergencies and rapid technological advances.

### Capabilities

Performing hazardous chemical analysis for emergency response.

Conducting mass spectrometry for elemental and isotopic signatures.

Designing field-portable instrumentation for biological and chemical detection.

Using optical spectroscopy for isotopic analysis.

Performing advanced, high-energy x-ray fluorescence for nuclear fuels.

Conducting materials analysis (surface, bulk, and particle).

### Technologies and Applications: Emerging, Developed, or Potential

- Synthesized a novel carboxyl-functionalized phosphonium room-temperature ionic liquid that could control the formation of solid-state uranium compounds. This type of ionic liquid has been proposed as electrolyte solutions that can be used for the electrodeposition of actinides during the reprocessing of nuclear fuels. Functionalized ionic liquids can address the low solubility of actinides by incorporating coordinating groups into the structure of the ionic liquid to promote complexation with uranium and plutonium.
- Developed a quick, fieldable method to detect live pathogens that can help detect hazardous bacteria in food supplies and thus help address public-health emergencies, such as major outbreaks of foodborne illnesses. The Los Alamos method eliminates the need for performing a laboratory culture and greatly speeds up the analysis process. This method uses bacterial siderophores to identify selectively and rapidly viable bacteria in their surroundings.
- Received accreditation from the American Association for Laboratory Accreditation for the Los Alamos Nuclear Forensic Analysis Center in the field of chemical

testing. Such accreditation involves bulk nuclear material analysis and is a key milestone for the Laboratory's nuclear forensics program. Los Alamos is one of two FBI "hub" laboratories for analyzing bulk special nuclear material. The FBI has in place a multi-laboratory network that assists criminal investigations related to planned or actual terrorist-driven nuclear attacks.

- Invested more than \$27 million in instrumentation and infrastructure for the Laboratory's mass spectrometry capability. Such instrumentation and infrastructure are dedicated to the analysis of inorganic, organic, biological, gas, solid, and liquid samples for elemental, isotopic, and structural information. Mass spectrometry in the area of chemistry enables researchers to measure trace and ultratrace elements within nuclear fuels. It also enables scientists to measure very low concentration of radionuclides, particularly those found in environmental samples. A combination of radiochemistry, mass spectrometry, and counting technology enable Los Alamos scientists to perform routine environmental monitoring in support of treaty verification and other threat-reduction missions.
- Use mass spectrometry is nearly all aspects of bioscience research, from analyzing small molecules to characterizing chemical-warfare agents to studying nucleic acids. In the area of biofuels, scientists are using mass spectrometry to identify the proteins and enzymes associated with the breakdown of cellulose. Metabolomic studies using stable isotopes and mass spectrometry enable a comprehensive understanding of growth in bacteria and algae, which is also useful for the development of new biofuels. Furthermore, these techniques are being used to identify transcription factors and other regulatory molecules.
- Used optical spectroscopy to study (1) semiconductors (both magnetic and nonmagnetic) based on GaAs, CdTe, ZnSe, GaN, and ZnO; (2) carbon nanotubes, (3) colloidal semiconductor quantum dots, (4) organic semiconductors that incorporate metal-porphyrine/phthalocyanine complexes, and (5) gold- and silver-based SERS nanosensors rapid biological and chemical detection.

#### Sponsors, Funding Sources, or Agencies

- [Department of Energy and National Nuclear Security Administration](#)
- [Department of Homeland Security](#)
- [Department of Defense and DTRA](#)
- [National Institutes of Health](#)
- Many others

#### Publications/Awards

N. Xu, L. Tandon, D. Gallimore, E. Lujan, D.R. Porterfield, L. Colletti, and K. Kuhn, "Dissolution and assay of neptunium oxide," *Journal of Radioanalytical and Nuclear Chemistry*, 1–5 (2012).

Kenneth G.W. Inn, C. Martin Johnson Jr., Warren Oldham, Simon Jerome, Lav Tandon, Thomas Schaaff, Robert Jones, Daniel Mackney, Pam MacKill, and Brett Palmer, et al., "The urgent requirement for new radioanalytical certified reference materials for nuclear safeguards, forensics, and consequence management," *Journal of Radioanalytical and Nuclear Chemistry*, 1–18 (2012).

Magen E. Coleman, Evelyn M. Bond, W. Allen Moody, and Lav Tandon, "The analysis of uranium-232: comparison of radiochemical techniques and an improved method by alpha spectrometry," *Journal of Radioanalytical and Nuclear Chemistry*, 1–5 (2012).

Steven C. Myers, Lav Tandon, Donivan R. Porterfield, Khalil J. Spencer, Mariam R. Thomas, and Patrick T. Martinez, "Gamma spectrometer measurements of microgram quantities of plutonium using uranium L X-rays in the 13-21 keV region," *Journal of Radioanalytical and Nuclear Chemistry*, 1–6 (2012).

Reid Porter, Christy Ruggiero, Don Hush, Neal Harvey, Patrick Kelly, Wayne Scoggins, and Lav Tandon, "Interactive image quantification tools in nuclear material forensics," *Proceedings of SPIE - The International Society for Optical Engineering*, 7877 (2011).

A. Pandey, S. Brovelli, R. Viswanatha, L. Li, J.M. Pietryga, V.I. Klimov, and S.A. Crooker, "Long-lived photoinduced magnetization in copper-doped ZnSe-CdSe core-shell nanocrystals," *Nature Nanotechnology* (2012).

N.A. Sinitsyn, Yan Li, S.A. Crooker, A. Saxena, and D.L. Smith, "Role of nuclear quadrupole coupling on decoherence and relaxation of central spins in quantum dots," *Physical Review Letters* 109(16) (2012).

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